

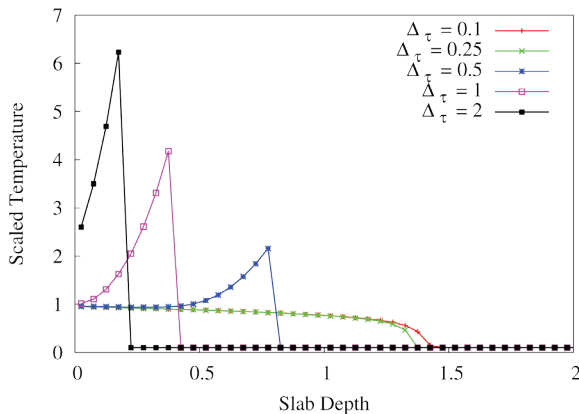
# A Discrete Maximum Principle for the Implicit Monte Carlo Equations

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Over forty years ago, the Implicit Monte Carlo (IMC) equations emerged as a robust linearization of the nonlinear thermal radiative transfer equations that describe the interaction of photons with matter. However, for sufficiently large time steps, the IMC equations can produce nonphysical “temperature spikes,” and the conventional remedy has been to manually reduce the time-step size until these artifacts disappear. We have derived necessary, sufficient, and approximate conditions on the time-step and temperature-grid sizes to ensure that the IMC temperature solutions satisfy a discrete maximum principle—that is, in the absence of inhomogeneous sources, the internal material temperatures remain between specified boundary conditions. This work is now being used as the basis of a dynamic time-step controller for the IMC equations.

The Implicit Monte Carlo (IMC) equations are an unconditionally stable time-discretization and linearization of the thermal radiative transfer equations that are amenable to a stochastic, particle-based (Monte Carlo) solution algorithm [1]. However, the IMC equations can admit nonphysical temperature solutions if the time step is chosen to be sufficiently large [2]. Specifically, for problems that contain no inhomogeneous sources, it has been shown that the thermal radiative transfer equations obey a maximum principle—that is, the interior temperatures are bounded above and below by the boundary condition temperatures at all times [3]. By contrast, if a sufficiently large time step is chosen, the IMC temperature solution can be made to exceed the boundary condition temperatures in a heating problem. Fig. 1 provides several examples of these IMC maximum principle violations. It depicts

Fig. 1. Temperature profiles at  $\tau=8$  for a Marshak wave problem in which the time step is varied using  $\Delta\tau=0.1, 0.25, 0.5, 1$ , and 2 mean free times for emission.



the spatial temperature profile of an initially cold material that is suddenly subjected to a hot, isotropic source of radiation on the left boundary at a dimensionless time of  $\tau=8$  using several different choices of time-step sizes. As the time-step size is increased, the maximum temperature of this Marshak wave increasingly overshoots the unit left boundary condition and retards the wavespeed.

Twenty-five years ago, Larsen and Mercier [2] provided a sufficient condition on the time-step size of the spatially continuous IMC equations to ensure that their solution does not violate the

maximum principle. However, their sufficient condition was considered too conservative for practical use, as simulations showed that time-step values that were orders of magnitude larger than their recommendation could be employed without the appearance of nonphysical temperature solutions.

Recently, we have developed new time-step restrictions to prevent nonphysical overheating that explicitly consider the spatial-grid size of the temperature discretization [4]. If the restriction on the time- and space-dependent grid parameters is satisfied, then we say that the IMC solution satisfies a discrete maximum principle. Our main approach is to approximately solve the IMC radiative-transfer equations, determine an estimate of the maximal radiation energy deposited in a mesh cell, and demand that the resulting temperature update not exceed the boundary temperature. This demand directly results in an approximate time-step recommendation such that the IMC equations do not violate the discrete maximum principle. Because our approach is approximate, we also developed rigorous necessary and sufficient conditions on the maximal time-step size. Employment of our approximate technique on sample problems thus far has provided highly accurate predictions of the grid-dependent, maximal time-step size for the IMC equations to admit physical solutions.

We tested our approach on a 1D, nonlinear, Marshak wave problem—an initially cold slab of material that is suddenly subjected to a hot, isotropic, temperature source on one boundary—using a wide range of spatial and temporal grid parameters and both frequency-dependent and grey (frequency-integrated) radiation descriptions in the Milagro

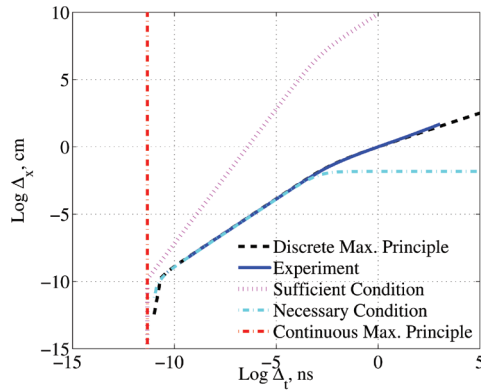


Fig. 2. First incidences of theoretically predicted (dashed) and experimental (solid) maximum-principle violations for a grey Marshak wave problem. The  $\Delta_T$  from the continuous maximum principle is the vertical line at the left.

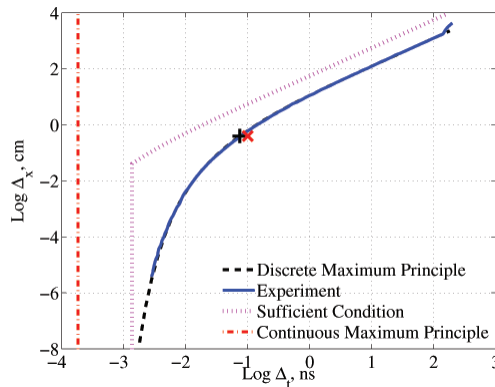


Fig. 3. First incidences of theoretically predicted (dashed) and experimental (solid) maximum-principle violations for a frequency-dependent Marshak wave problem.

IMC code [5]. The grey results are depicted in Fig. 2 on a log-log scale in which the abscissa measures the time-step size and the ordinate the spatial grid size. The solid blue curve indicates interpolated numerical results of IMC calculations that segregate physical solutions (above and to the left of this line, corresponding to small time steps and large spatial cells) and nonphysical solutions (below and right of this curve, corresponding to large time steps and small spatial cells). The black, dashed curve represents the critical time-step sizes predicted by our approximate technique. These exhibit excellent agreement. Additionally, they are

bounded above and below by the rigorous sufficient and necessary conditions that we developed (dashed magenta and dot-dashed cyan lines, respectively). Finally, we note that the vertical red line corresponds with the grid-free recommendation of Larsen and Mercier [2], which can be many orders of magnitude smaller than the observed value depending on the chosen time-step size. Figure 3 depicts the results of the same experiment when frequency-dependent opacities are incorporated, which necessitated the development of more involved approximations [4]. Again, our approximate prediction (the black, dashed curve) is in excellent agreement with interpolated numerical results from many IMC simulations (the solid blue curve). The necessary condition is not shown, as it was always satisfied for this problem. Figure 3 also depicts two data points from Larsen and Mercier's earlier work, the black "plus" sign, corresponding to an IMC calculation without maximum principle violations, and the red "x," corresponding to a nonphysical solution. Because the left plus sign is about three orders of magnitude larger than the predicted time-step limit, Larsen and Mercier remarked that their time-step limit was too conservative.

However, Fig. 3 shows that their choice of the spatial grid size had a substantial influence on that assessment.

Because the memory requirements of the numerical solution of the IMC equations are significant, it has been computationally prohibitive to adaptively restart an IMC calculation from the previous cycle using a smaller time step whenever maximum principle violations are encountered. Using our theory as its foundation, research is now underway to construct an inexpensive, grid-dependent, dynamic time-step controller for the IMC equations that should preclude nonphysical temperature spikes in the IMC temperature solution. Paul W. Talbot of Oregon State University has undertaken the 3D extension and implementation of this work into Jayenne Project software as part of his Master's project [6].

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